Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions

At the Abdus Salam International Centre for Theoretical Physics

BOOK OF ABSTRACTS

Trieste, Italy from 4-8 February 2008

	Monday		Tuesday		Wednesday		Thursday		Friday	
	INC models	Chair: D. Filges	INC/PE models	Chair: S. Leray	QMD models	Chair: J. Cugnon	De-excitation models	Chair: S. Mashnik	De-excitation models	Chair: Y. Yariv
9:00 -9:45			CEM03.03 and LAQGSM03.03 Event Generators for MCNP6, MCNPX and MARS15	S. Mashnik (LANL, USA)	The Description of Nuclear Collision within the Quantum Molecular Dynamics Model	C. Hartnack (Subatech, France)	The Role of Multifragmentation in Spallation Reactions	A. Botvina (INR, Russia)	The de-excitation code ABLA07	K.H. Schmidt or A. Kelic (GSI, Germany)
9:45 -10:30	Introduction and Aim of the Meeting	D. Filges (FZJ Jülich)								
Coffee Break										
11:00-12:30	ISABEL - INC Model for High-Energy Hadron-Nucleus Reactions	Y. Yariv (Soreq, Israel)	models in FLUKA	A. Ferrari (INFN, Italy)	Nuclear Reaction Models (JAM and JQMD) in PHITS	K. Niita (RIST, Japan)	GEMINI: Dexcitation of excited compound nuclei through a series of binary decays	R. Charity (or L. Moretto, USA)	GEM	To be decided
Lunch										
14:00 -14:45	Detailed description of the Intra Nuclear Cascade from Liege: INCL4	A. Boudard (CEA, France)	Proton induced spallation reactions investigated within the framework of BUU model	Z. Rudy (Krakow)	Experimental data on evaporation and pre-equilibrium emission in GeV p-induced spallation reactions	F. Goldenbaum (FZJ, Germany)	ITEP experiments with thin targets irradiated by upto 2.6 GeV protons	Y. Titarenko (ITEP, Russia)	Summary and perpectives (intercomparison description)	S. Leray (CEA, France)
14:45-15:30			Neutron Data	To be decided	Detailed Investigation of Residual Nuclei Produced in Spallation Reactions at GSI	J. Benlliure (Santiago univ., Spain)	Experimental Cross Sections for the Production of Residual Nuclides at Medium Energies: Status, Recent Progress and Challenges for Modeling	R. Michel (Uni Hannover, Germany)		
Coffee Break										
16h00 - 18h00	General Meeting	Goals of the intercomparison	Expert meeting on intercomparison	Choice of experimental data (including Neutron Data)	Expert meeting on intercomparison	Figures of merit	Expert meeting on intercomparison	Data and results format, general discussion	Closed session (Report)	Directors
	Spallation Data and Applications	A. Mengoni, A. Stanculescu (IAEA)								
Dinner										
20:30 - 21:45	Reception		Discussion		free		Evening event			free

Introduction and Aim of the Meeting

Detlef Filges

Institut für Kernphysik
Forschungszentrum Jülich GmbH
D-52425 Jülich, Germany

Particle transport in matter became an increasing importance in many fields of basic science, technology and applications in the recent years. The investigation of hadronic and electromagnetic cascades is of considerable interest for all aspects of radiation physics. With the advent of high intensity spallation neutron sources with a proton beam power in the MW range e.g. SINQ- Switzerland, SNS-USA, JPARC-Japan, with research projects e.g. a long pulsed European Spallation Neuron Source (ESS), -The European Roadmap for Research Infrastructures-, Accelerator Driven Systems (ADS) for nuclear waste transmutation and energy production , with the application of radioactive beams, with the detectors and experiments at medium and high energy accelerators, and with cosmic and space applications detailed particle production and transport models realized in computer code systems have to be used to demonstrate feasibility and utilization, to optimize the design configurations, and to support the engineering layout. The talk summarizes the currently state-of-the-art particle transport simulation code systems used in spallation research and in particle transport through matter and gives a short tabulated overview which spallation reactions models are in use and are the base of this workshop.

ISABEL - INC MODEL FOR HIGH-ENERGY HADRON-NUCLEUS REACTIONS

Yair Yariv

Soreq, NRC, Yavne 81800, Israel

Basic assumptions of the INC models are "revisited" in order to examine their applicability limits at low energies. A detailed description of the INC Monte Carlo code ISABEL developed in 1978-1980 is given with emphasis on the physical assumptions, actual implementation and parameters.

Detailed description of the Intra Nuclear Cascade from Liège: INCL4

A. Boudard

CEA-Saclay, DSM/LSCE/LMC14, Bat. 450
91191 Gif sur Yvette, FRANCE

The "Intra Nuclear Cascade from Liège" appeard more than 25 years ago.

It's originality lies in an explicit treatment of all the particles in a classical picture and as a function of time. It has been continuously developed and improved to end up presently with the version INCL4 of the code.

The various physical ingredients used in the most recent version and their explicit implementation will be presented with a discussion of all parameters and of the influence on observables.

Intranuclear cascade evaporation model: critical comments

A.Yu. Konobeyev, U. Fischer,

Institut für Reaktorsicherheit, Forschungszentrum Karlsruhe GmbH,
Postfach 3640, 76021, Karlsruhe, Germany

Various modifications of intranuclear cascade evaporation are analyzed. Advantages and lacks of modern approaches and approximations are demonstrated. The combination of the intranuclear cascade model and the equilibrium model with approximate and accurate description of the angular momentum is discussed.

CEM03.03 and LAQGSM03.03 Event Generators for MCNP6, MCNPX, and MARS15 Transport Codes

S. G. Mashnik1, K. K. Gudima2, R. E. Prael1, A. J. Sierk1, M. I. Baznat2, N. V. Mokhov3

1Los Alamos National Laboratory, Los Alamos, NM 87545, USA
2Institute of Applied Physics, Academy of Science of Moldova, Chi¸sin˘au, Moldova
3Fermi National Accelerator Laboratory, Batavia, IL, USA

A detailed description of the IntraNuclear Cascade (INC), preequilibrium, evaporation, fission, coalescence, and Fermi breakup models used by the last version of our CEM03.03 and LAQGSM03.03 event generators is presented, with a focus on our latest development of all these models. The recently developed "S" and "G" versions of our codes, that consider multifragmentation of nuclei formed after the preequilibrium stage of reactions when their excitation energy is above 2A MeV using the Statistical Multifragmentation Model (SMM) code by Botvina et al. ("S" stands for SMM) and the fission-like binary-decay model GEMINI by Charity ("G" stands for GEMINI), respectively, are briefly overviewed as well. Examples of benchmarking our models against a large variety of experimental data on particle-particle, particle-nucleus, and nucleus-nucleus reactions are presented. Open questions on reaction mechanisms and future necessary work are outlined. This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

Proton induced spallation reactions investigated within the framework of BUU model

Zbigniew Rudy

Jagellonian Univ., Krakow, Poland

Major progress of contemporary research in the natural sciences can no longer be imagined without model simulations. Particularly demanding are cases when one wants to investigate a real dynamic system. The simulation of nuclear reaction form such a case where one is compelled to introduce essential simplifications in order to make truly quantum N-body problem calculable. Sure, the simplifications should be chosen carefully, if not they can distort the time evolution of dynamic system. Essential for nuclear reaction is diffusion of interacting particles, therefore it is natural to expect that approach based on Boltzman equation of transport is promising one. The Boltzmann-Uehling-Uhlenbeck model, which includes Fermi motion of nucleons, the mean field of their interaction, individual N-N interactions and quantum mechanical Pauli blocking effect can be used for calculations of properties of hot residual system – its distributions of excitation energy, mass, charge and angular momentum. Such a model will be presented in the talk, starting from derivation of transport equation. The ingredients of the model will be discussed with stress put to deficiencies they impose. E.g. feasibility of the collision term of the transport equation which is constructed in specific way in order to respect the Pauli blocking is well justified, however, test particle method used for one body phase space density of the nucleons requires sufficiently large number of test particles. It will be shown how the BUU model supplemented with statistical evaporation code (i.e. statistical evaporation code as "afterburner" of hot residual nuclei) describes the sample data.

The description of nuclear collision within the Quantum Molecular Dynamics model

Christoph Hartnack

SUBATECH, UMR 6457 Ecole des Mines de Nantes, IN2P3/CNRS, Nantes University 4, rue Alfred Kastler, F-44307 Nantes, Cedex 03, France

The QMD model (quantum molecular dynamics) is a semiclassical microscopic model for the description of nucleus-nucleus collissions on an event-by event level. The basic features of the QMD- model and the differences (and common parts) of different implementations (BQMD, IQMD, UrQMD) will be presented.

The basic ingredients in the description of the initialisation, potential propagation and collision part will be described and their influence to physical observables will be discussed.

Nuclear Reaction Models (JAM and JQMD) in PHITS

Koji Niita

Research Organization for Information Science & Technology,
Tokai, Ibaraki, Japan

The cross sections of intermediate and high energy nuclear reactions are strongly required in design study of many facilities such as accelerator-driven systems, intense pulse spallation neutron sources, and also in medical and space technology. There is, however, few evaluated nuclear data of intermediate and high energy nuclear reactions. Therefore, we have to use some models or systematics for the cross sections, which are essential ingredients of high energy particle transport code to estimate neutron yield, heat deposition and many other quantities of the transport phenomena in materials.

In the particle and heavy ion transport code system PHITS, we have used two simulation codes JAM and JQMD to describe the intermediate and high energy nuclear reactions

JAM (Jet AA Microscopic Transport Model) is a simulation code based on INC (intra-nuclear cascade) model, which explicitly treats all established hadronic states including resonances with explicit spin and isospin as well as their anti-particles.

We have parametrized all hadron-hadron cross sections based on the resonance model and string model by fitting the available experimental data.

JQMD (JAERI Quantum Molecular Dynamics) is a simulation code based on the molecular dynamics. A typical feature of QMD compared with that of the INC model is that QMD can describe not only nucleon-nucleus reactions but also nucleus-nucleus reactions in the same framework. Though the QMD model have been used mainly for the heavy-ion physics, we have applied JQMD code intensively to nucleon-nucleus reactions and checked its validity.

In this lecture, physical ideas and the details of these two models are discussed. In addition to these two models, which describe the dynamical stage of the reactions, we have to combine these models to the statistical decay models in order to obtain the cross sections of the final ejectiles of the reactions. The features of the connection of dynamical and statistical models are also discussed.

Experimental data on evaporation and pre-equilibrium emission in GeV p-induced spallation reactions

Frank Goldenbaum

Forschungszentrum Jülich GmbH,
52425 Jülich, Germany

The contribution will focus on the latest progress on nuclear data measured by the experiments PISA and NESSI performed at the COoler SYnchrotron COSY in Juelich, Germany. The objective of the measurements is to provide reliable and comprehensive experimental data serving as benchmarks for code development and validation in the 200-2500 MeV energy range. To scrutinize the codes under consideration on this workshop and to calculate as reliably as possible quantities related to high energy reactions, hadronic interaction lengths, reaction cross sections, average particle multiplicities, particle multiplicity and double differential energy/angular distributions need to be investigated. In this presentation the latest results of PISA and NESSI experiments essentially on hydrogen- and helium isotopes, intermediate mass production, but also on neutron multiplicities will be given.

Detailed Investigation of Residual Nuclei Produced in Spallation Reactions at GSI

J. Benlliure

Universidad deSantiago de Compostela, Spain

The production of residual nuclei in spallation reactions has been widely investigated at GSI (Darmstadt) using inverse kinematics and the magnetic spectrometer Fragment Separator (FRS). This experimental technique has allowed for the isotopic identification of all residual nuclei produced in these reactions with half-lives longer than 200 ns and the determination of their production cross sections and momentum distributions with high accuracy. The large data collection obtained in these experiments can be used for detailed benchmarking of physics models describing these reactions. In this talk we will present the experimental technique, the data reduction method and some of the most salient results.

The Role of Multifragmentation in Spallation Reactions

A.S. Botvina

Institute for Nuclear Research, Russian Academy of Sciences, Moscow, Russia)

In nuclear reactions induced by hadrons and ions of high energies, nuclei can disintegrate into many fragments during a short time (~100 fm/c). This phenomenon known as nuclear multifragmentation was under intensive investigation last 20 years. It was established that multifragmentation is an universal process taking place in all reactions when the excitation energy transferred to nuclei is high enough, more than 3-4 MeV per nucleon, independently on the initial dynamical stage of the reactions. Very known compound nucleus decay processes (sequential evaporation and fission), which are usual for low energies, disappear and multifragmentation dominates at high excitation energy. For this reason, calculation of multifragmentation must be carried on in all cases when production of highly excited nuclei is expected, including spallation reactions. From the other hand, one can consider multifragmentation as manifestation of the liquid-gas phase transition in finite nuclei. This gives way for studing nuclear matter and for other applications in astrophysics.

In this lecture, the Statistical Multifragmentation Model (SMM), which combines the compound nucleus processes at low energies and multifragmentation at high energies, is introduced, and comparison with adequate experimental data is demonstrated. The most effective ways for description of the whole reaction, and the most crucial observables, are discussed.

GEMINI: Dexcitation of excited compound nuclei through a series of binary decays.

Robert Charity

Washington University, St. Louis, USA

The code GEMINI represents the implementation of a general binary decay mode of the compound nucleus as suggested by Moretto with explicit treatment of angular momentum effects. This includes light-particle evaporation in the limit of the most asymmetric divisions and fission for the other limit. In addition all intermediate asymmetries are allowed. The justifications of the formalism are discussed at length. However there are theoretical uncertainties in the implication of this formalism that require calibration of the model in each mass region. The model as presently implemented in GEMINI is shown to be most appropriate for light compound nucleus. In heavy compound nuclei, the predicted fission-fragment mass distributions are too large. Modifications of fission mass distribution by the saddle-to-scission motion and by the Wigner energy are discussed as well as recent changes to the code to address this.

ITEP experiments with thin targets irradiated by upto 2.6 GeV protons

Authors: Yury E. Titarenko, Viacheslav F. Batyaev

I.T.E.P., B. Cheremushkinskaya ul. 25, 117259 Moscow
RUSSIAN FEDERATION

Preliminary Abstract: A detailed review of the thin target experiments made on the ITEP (Moscow) proton synchrotron during last decade is given. The experiments were aimed to determination of independent and cumulative yields of radioactive residual product nuclei in thin targets induced by 0.04-2.6GeV protons.

144 targets of 22 materials from ^{nat}Cr to ^{nat}U have been irradiated by the moment. The preference was made to isotopic enriched materials such as isotopes of lead (^{206}Pb, ^{207}Pb, ^{208}Pb), iron (^{56}Fe), tungsten (^{182}W, ^{183}W, ^{184}W, ^{186}W), technetium (^{99}Tc). In total, more than 10000 yields had been determined in the experiments by 2005 and published in available reports and EXFOR database. The new set of data on structure materials (^{56}Fe, ^{nat}Cr, ^{nat}Ni, ^{93}Nb, ^{181}Ta, ^{nat}W) is being processed and is to be finished in 2009.

The presentation will provide also a description on experimental methods used, the techniques and results of comparison with predictions by simulation codes, and results of comparison with other experimental data obtained mainly at GSI(Darmstadt) and ZSR (Hannover).

Experimental Cross Sections for the Production of Residual Nuclides at Medium Energies: Status, Recent Progress, and Challenges for Modeling

Rolf Michel

Zentrum für Strahlenschutz und Radioökologie, Leibniz Universität Hannover,
Herrenhäuser Str. 2, D-30419 Hannover, Germany

The production of stable and radioactive residual nuclides by medium-energy protons and neutrons is of importance for many fields of basic and applied sciences ranging from astrophysics over space and environmental sciences, medicine, accelerator technology, space and aviation technology to accelerator driven transmutation of nuclear waste and energy amplification. In this contribution, recent achievements and some still open questions in the understanding of nuclide production at medium energies are discussed. Starting from the 1997 NEA International Codes and Model Intercomparison for Intermediate Energy Activation Yields, the suitability of new data sets for an advanced intercomparison is discussed. Such an intercomparison should allow testing the overall performance of model codes for a wide variety of target elements, particle energies, and reaction modes. It should demonstrate the capabilities of codes to handle at least protons, neutrons and light nuclides in the entrance channel. Particular reactions are proposed to test some extremes of nuclear reactions. Possible candidates for testing the performance of model codes are thin-target data for proton-, alpha-, and neutron-induced reactions with respect to individual nuclear reactions as well as thick-target data with respect to the overall capability of models to describe secondary particle production, particle transport and radionuclide production.

The de-excitation code ABLA07

A. Kelic and K.-H. Schmidt

Gesellschaft für Schwerionenforschung, GSI, Darmstadt, Germany

The modelling of spallation reactions is usually done in two reaction steps: The first stage, beginning at the first contact of the incoming particle with the target nucleus is most often described by an intra-nuclear-cascade code. In a sequence of nucleon-nucleon collisions, the heavy remnant of the target developes towards an intrinsically equilibrated nuclear system, while a number of particles and light fragments leave the system. The equilibrated heavy system is fully characterized by its composition in mass and atomic number and by its linear and angular momentum.

These are the conditions at the beginning of the decay of the excited system, which is most appropriately described by a dedicated de-excitation code. Most of the characteristics of the final nuclide yields, e.g. their distribution on the chart of the nuclides and signatures of fine structure, are dominantly determined by this second reaction stage.

Traditionally such codes considered only the most important exit channels: evaporation of neutrons, protons and alpha particles as well as fission within the statistical model. While the residues close to the target nucleus were rather well reproduced, large discrepancies were observed in other regions. Comparison with recent experimental data has revealed that several features have to be carefully considered for obtaining a satisfactory description of the deexcitation process:

1. Expansion and spinodal instabilities of the hot compound, eventually leading to multifragmentation.
2. Binary decay in all possible splits, from the evaporation of nucleons to symmetric fission.
3. Dynamics of the shape evolution towards fission, suppressing the fission channel at early times.

In addition, the realistic description of the mass and nuclear-charge split in fission, in particular at low excitation energies, where distinct structural effects appear, appears to be very challenging.

Modern de-excitation codes have tackled these problems with different strategies, focussing their main efforts on different features. Besides the most realistic model description, a moderate expense in computing time constitutes another important criterion.

The development of ABLA07 has been guided by the empirical knowledge obtained in a recent experimental campaign on the nuclide distributions formed in the spallation of a number of systems at GSI, Darmstadt. Besides distinct signatures of very asymmetric binary spits, lighter systems show clear features of multifragmentation, while heavy systems reveal the influence of dynamics and microscopic structure on the fission process. ABLA07 includes elaborate but efficient descriptions of all the processes mentioned above. Large effort has been invested in the most realistic description of the fission process. Transient effects and the descent from saddle to scission are modelled with analytical approximate solutions of Langevin calculations. Residual nuclide distributions are calculated with a macro-microscopic approach, considering the influence of compound-nucleus and fragment properties on the fission path.

The presentation will focus on:

- demonstrating the experimental signatures of the different features,
- discussing the basic physics behind the empirical phenomena, and
- documenting the main features of the model description.